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Bonding, Energetics and Mechanical Properties of Intermetallics

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Contents

Abstract	1
I Background Perspective	2
II Accomplishments/New Findings	2
1 Method Developments	2
1.1 Ab-initio electronic structure calculations	3
1.1.1 FLAPW method with atomic force capabilities	4
1.1.2 FLMT0 method with structural optimization capabilities	4
1.1.3 Combination of the real-space tight-binding LMTO method with the re- cursion method	5
1.2 Methods for multi-scale modeling and simulations	6
1.2.1 General scheme for solving the Peierls-Nabarro model with a two com- ponent displacement field and restoring forces determined from ab-initio generalized stacking fault energetics.	6
1.2.2 Determination of the dislocation dissociation "path" within a 2D PN model analysis.	7
2 First-principles determination of the universal parameters controlling brittle to ductile behaviour.	7
2.1 Cleavage and slip energy barriers for B2 NiAl and FeAl (FLAPW study).	8
2.2 Planar shear and cleavage decohesion processes in NiAl and FeAl (FLMT0 study).	8
3 Ab-initio generalized stacking-fault energetics and properties of dislocations: 1D and 2D PN model analysis with generalized restoring force law	10
3.1 Dislocation structure and mobility in B2 FeAl and NiAl: 1D PN model analysis with ab-initio GSF energetics.	10
3.2 Ordinary dislocation properties in TiAl vs. CuAu: Peierls-Nabarro model with two component displacement fields and generalized restoring force law.	11
4 Real-space tight-binding-linear-muffin-tin orbital method investigation of point and extended defects in intermetallics.	13
4.1 Preferable site energies of impurities in NiAl.	13

4.2	First-principles calculation of the electronic structure of dislocations: screw and edge dislocations in NiAl.	13
5	First-principles calculations of the size misfit parameters for various impurities in NiAl.	14
6	References	16
III	Publications supported by AFOSR	20

Abstract

The objective of this research was to investigate fundamental aspects of the fracture and deformation behavior of ordered intermetallic aerospace alloys on the basis of the ab-initio determination of the parameters needed for further (i) model theoretical, (ii) band structure and (iii) chemical bonding analyses. The research was targeted at investigating the microscopic mechanisms governing the deformation and fracture behavior of intermetallic alloys in order to contribute to the development of a fundamental basis for computer-aided alloys design. Progress in this complex area required understanding such key phenomena as dislocation structure and mobility, and crack blunting and propagation: while they have been characterized by mesoscopic length and energy scales, they are determined on the microscopic level by the electronic structure. Thus, this most important and challenging component of our research was to bridge the gap between a microscopic quantum-mechanical description of the chemical bonding and the mesoscopic phenomena which govern the mechanical response of intermetallics. Especially for intermetallic compounds and metals of interest, we concentrated on (i) fundamental aspects of dislocation structure and mobility; (ii) solid-solution hardening problems in the context of the fundamental aspects of impurity-dislocation interaction theory; (iii) the electronic structure of dislocations and related properties of real crystals. These important, complex problems required the use of a hierarchy of methods. We focussed on the application and further development of both state-of-the-art band structure and real-space large scale cluster electronic structure methods which provide parameters needed for atomistic simulations and model mesoscopic simulations. In this way, we greatly amplified the impact of our research based on our quantum-mechanical electronic structure simulations.

Part I

Background Perspective

It is now clear that the high temperature intermetallics have become a major focus of research effort – both experimental and theoretical – driven in large part by their potential for important aerospace applications. In the theoretical area of this research, our work (initiated and carried out under AFOSR support), has been at the forefront and has already stimulated similar efforts at other laboratories. The present state of the field has reached a threshold: advanced theoretical-computational techniques combined with the power of supercomputers provide an understanding of matter at the atomic-scale with an unprecedented level of detail and accuracy. It is this capability that has given birth to a new branch of scientific endeavor: Computational Materials Science. In contrast to an analytic-theoretical approach, which isolates and idealizes real systems to unravel fundamental relations and laws, the computational approach is synthetic: its goal is to simulate more and more details (i.e., complexity) of the systems studied including as much of the environment as possible. It thus provides materials scientists and engineers fine details on specific systems, rather than rules of thumb for all systems. This is now recognized as the emerging power of computational science, and ultimately computational materials design.

Today, theoretical efforts are focused on the atomic scale and the theoretical concepts and methodologies being developed are bringing us closer to the goal of a unified approach for calculations on a nano and submicron scale. The theoretical approach, density functional theory, that underlies all the calculations discussed here is appealing because it promises to provide such a unified approach, which is particularly suited for bridging the gap between our understanding of atomic scale properties and the macroscopic properties essential for producing useful materials applications.

Part II

Accomplishments/New Findings

1 Method Developments

The mechanisms of the ductile/brittle behaviour and anomalous mechanical response of inter-metallic aluminides are still far from being well understood and remain a challenge to theoretical

explanation. This problem seems to be extremely difficult since accurate, microscopic descriptions of the directional covalent chemical bonding are required for modeling the mesoscale phenomena (dislocations).

1.1 Ab-initio electronic structure calculations

Since a key feature of our approach is an accurate description of the interatomic interaction, based on ab-initio electronic-structure, we briefly describe and illustrate several first-principles methods with their different features and functionality. We emphasize the importance of employing different electronic structure methods to meet the requirements of these complex material science problems, especially ones related to mechanical properties and fracture. It is important also to stress here that the fundamental basis of ab-initio methods is density-functional theory (DFT); this is a practical way to treat the many-electron problem within fundamental quantum mechanical principles. This theory has proved, over two decades, to be a general, predictive approach for addressing various problems of computational materials science.

In principle, to describe the properties of solids, DFT does not require any additional information other than the atomic number of the component elements. However, computational limitations (basically aspects related to the use of appropriate numerical algorithms) are the reason why only relatively few materials can be treated without making any additional simplifications. In the case of an ideal periodic crystal, an infinite number of atoms can effectively be taken into account through the use of Bloch's theorem to treat a basic unit cell.

Different ab-initio techniques can be characterized by how the space is partitioned and by the set of basis functions employed. The most widely used electronic structure methods are: (i) the full-potential linearized augmented-plane-wave method (FLAPW) [1], (ii) the linear-muffin-tin-orbital method (LMTO) [2, 3, 4] and (iii) molecular cluster methods like DMol [5, 6]. The first two belong to a large class of energy band methods, or methods that rely on Bloch's theorem, and the third represents so-called real-space approaches.

Another important functionality of these methods is the capability to find atomic structures corresponding to a minimum of the total energy. The most efficient way to perform this minimization with respect to atomic degrees of freedom is to determine interatomic forces directly from the calculated electron band energy spectra and wave functions.

An overview of the different ab-initio local-density computational methods can be found in Ref. [7] along with references to the original works. Here, we briefly characterize the methods (and some of our developments) used in our study of the mechanical properties of materials.

1.1.1 FLAPW method with atomic force capabilities

The ability to calculate atomic forces has been implemented into the present version of the total energy FLAPW code. An automatic optimization procedure searches for the optimal structure. For a self-consistent structure the total energy and the forces on all atom are calculated. For n atoms this gives an $3n$ dimensional force-vector. An automatic optimization procedure moves all atoms simultaneously until a configuration of the system is found for which the $3n$ dimensional force-vector is zero. This allows the relaxation of rather complex systems with high precision. The automatic optimizer can operate in two different modes: (i) a self-scaled Broyden method for function minimization and (ii) a molecular dynamics approach with a damped Newton method in which the time step is replaced by the iteration index. Both methods are in general suitable to find the optimum geometry of the system. Method (i) relies on the validity of a quadratic expansion of the total energy around the equilibrium structure, and thus can fail if this is not justified. In a sense, Method (ii) merely follows the Newton equation and therefore can find an optimized structure in those cases where method (i) fails.

In addition, the full dynamical matrix of an optimized structure can be calculated. This allows the determination of the phonon spectrum of the system, without any further model assumptions in determining the various eigen-modes. The dynamical matrix is defined as

$$D_{i,j} = \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 E}{\partial x_i \partial x_j}, \quad (1)$$

where m_i and x_i are the mass and the position of the i -th particle and E is the total energy of the system. Since the forces are calculated from an analytic expression derived for the FLAPW method, one can rewrite Eq.(1) in terms of forces. The resulting expression

$$D_{i,j} = -\frac{1}{\sqrt{m_i m_j}} \frac{\partial F_i}{\partial x_j} \approx -\frac{1}{\sqrt{m_i m_j}} \frac{\Delta F_i}{\Delta x_j} \quad (2)$$

is solved in a finite differences approach. The eigenvalues and eigenvectors of the matrix D_{ij} give the phonon spectrum of the system under consideration.

1.1.2 FLMTO method with structural optimization capabilities

The implementation of an analytical force formalism in the present formulation of the full-potential linear muffin-tin code (FLMTO) is a complicated task. Therefore, we implemented the numerical force formalism based on the Harris-Foulks functional. The main idea of the method is to obtain self-consistently the total energy of a system and then, starting from the self-consistent charge density, to estimate the total energy of the infinitesimally distorted system

using the Harris-Foulks functional in a single iteration. From this, the force on a chosen atom can be calculated by numerical differentiation of the total energy. Of course, the main drawback of this approach is that one has to specify an atom for which the force is to be calculated, but usually in all band structure approaches there are strict limitations, from the symmetry of the unit cell, on those atoms that are allowed to relax.

The FLMTO method itself is fast enough so that several additional iterations (to find forces) result in only a minor impact on the total time of the calculations. After the numerical forces are calculated one can proceed with the structural optimization. Phonon frequencies can be calculated in a slightly different way than described above. Since the forces can be calculated only for specific atoms it is impossible to set up the whole dynamical matrix. On the other hand, one can find irreducible representation of the dynamical matrix using symmetry considerations. In this case the dynamical matrix would split into different "phonon modes". Each of these phonon modes (representing only the atomic displacements connected by symmetry) can be calculated separately in a way similar to the above.

1.1.3 Combination of the real-space tight-binding LMTO method with the recursion method

The specific features of the materials science problems related to mechanical properties require large-scale simulations of extended defects or phenomena that are characterized by mesoscopic length and energy scales. The electronic-band-structure supercell and traditional cluster-real-space methods are not quite satisfactory for simulating such situations, both because of the limited number of atoms that can be handled and the boundary conditions these techniques allow one to employ.

To better meet these special requirements for theoretical studies of mechanical behaviour, we have adapted and coded the first-principles real-space technique TB-LMTO-REC which combines the TB-LMTO [8, 9] formalism for the real-space one-electron Hamiltonian and the recursion method to calculate the resolvent operator [10]. We follow the TB-LMTO scheme proposed by Andersen [8, 9], as described in Ref. [11], where we demonstrated the superiority of the TB-LMTO- Hamiltonian over the empirical tight-binding model, described details of the implementation, and presented test results that demonstrated that real space TB-LMTO calculations can be carried out without serious loss of precision compared to the conventional LMTO band method. This technique was later used to study the magnetism of amorphous iron and impurity effects in bcc Fe [12, 13]

The real-space nature of this method and the efficient resolvent operator [10] technique allows one to describe in a most appropriate, but still feasible, way both the core and the long range elastic stresses of dislocations. The method allows us to simulate very low doping, which

is not accessible by electron energy band techniques. Due to the numerical efficiency and high (linear) scalability of the method, the region of self-consistent treatment may be taken to be very large (i.e., to contain hundreds of atoms) with tens of thousands of atoms in whole clusters to minimize surface effects.

1.2 Methods for multi-scale modeling and simulations

1.2.1 General scheme for solving the Peierls-Nabarro model with a two component displacement field and restoring forces determined from ab-initio generalized stacking fault energetics.

A general scheme for analyzing the structure and mobility of dislocations is based on solutions of the Peierls-Nabarro model with a two component displacement field and restoring forces determined from the ab-initio generalized stacking fault energetics (ie., the so-called γ -surface). The approach allows one to establish an explicit relation between quantities which can be accurately determined using microscopic quantum mechanical methods (γ -surface) and dislocation properties (processes approaching mesoscopic scales). As we demonstrated (see below), a unified description of compact, spread and split dislocation cores is provided with an important characteristic "dissociation path" revealed by this proposed highly tractable scheme. We used this method to determine the structure and Peierls stress of the single dislocation for L10 TiAl, CuAu, fcc Ir and Au.

Despite its well-known approximations [14, 15, 16, 17], the PN model is very attractive since it offers a tractable description with parameters (γ -surface) accessible by highly accurate quantum mechanical calculations [18, 19]. As was recently demonstrated, the applicability of the Peierls model framework can be extended in a semi-discrete version even for such an extreme case as narrow dislocation cores in Si [15]. Unfortunately, the proposed semi-discrete scheme [15] is purely numerical; however, in the theory of such complex lattice defects as dislocations, it is highly desirable to keep the high tractability of the theoretical approach as much as possible.

To date, the PN model analysis with first-principles parametrization for GSF energetics was restricted, however, to considering dislocations with a single component displacement field (one dimensional (1D) PN model) in Si [20] and in B2 intermetallic compounds [18]. The abilities of the PN model to deal with dislocation cores in intermetallics has not yet been studied systematically, except for our earlier overall encouraging experience with the 1D-PN model for dislocations in B2 NiAl and FeAl [18]. However, the two component displacement field (two-dimensional (2D) PN model), with the possibility of dislocation dissociation; is quite a typical situation in general and, in particular is necessary to be considered in the case of unit dislocations for L1₀ TiAl and CuAu, materials with similar fcc-like structure but very different

mechanical behaviour.

In contrast with the 1D PN model, exact solutions of the 2D-PN model are unknown even for the simplest sinusoidal restoring force law. Recently, Schoeck presented a direct variational method for analyzing, on the energy functional level, the 2D-PN model using ansatz solutions with geometric parameters [21]. This method has been used to calculate dislocation core structures corresponding to model GSF surfaces [22]. We proposed an alternative scheme for solving 2D-PN model equations within a wide class of analytic functions which makes this scheme unified (i.e., free of parameters and assumptions on dislocation structure), suitable for analyzing realistic/complex γ -surfaces and physically transparent. We demonstrated that this proposed approach explains qualitative differences in dislocation structure and mobility in a very natural way and establishes an explicit relation between γ -surface geometry and dislocation properties within the 2D PN model. This allows one to relate GSF energetics determined from ab-initio electronic structure calculations with dislocation structure using a unified and highly transparent procedure.

1.2.2 Determination of the dislocation dissociation "path" within a 2D PN model analysis.

In contrast with the screw, the maximal value of the edge component is unknown in fcc lattices. Usually, it is assumed to be determined by the position of the CSF which may be justified only in the limit of large splitting distances. In this limit, dependence of the screw on edge displacement components $u_2 = f(u_1)$ or "dissociation path" may be well approximated by a straight line (assumed "dissociation path"). Scheme proposed for solving coupled 2D PN model equations procedure proposed to handle coupling of the 2D PN model equations allows us to also find the actual "dissociation path", curve $u_2 = f(u_1)$ determined using iterative procedure with straight "path" used as a trial[23]. We would like to emphasize here importance of this finding revealed due to high tractability of the proposed scheme for 2D PN model analysis. The possibility of such a transition from the split/spread to compact solution (with a corresponding transformation of the "dissociation path") has also been recently indicated by Schoeck in a 2D PN model analysis with model type γ -surfaces using the direct variational approach [22].

2 First-principles determination of the universal parameters controlling brittle to ductile behaviour.

The principal processes that determine brittleness/toughness are dislocation mobility and crack blunting [24]. In the case when the effects of crack shielding can be neglected (for example when

the mobility of the dislocations is low), the description of brittle vs. ductile behaviour in terms of the Rice-Thompson approach [24, 25, 28, 26] is based on a comparative analysis of two competing processes: (i) the opening of the crack and (ii) the emission of a dislocation near the crack tip. Now, the resistance to dislocation emission at a crack tip may be measured by the maximum energy associated with the sliding of atomic planes [28]. This parameter, the so called unstable stacking fault energy (γ_{us}), is determined by extremal properties of the γ -surface, namely, the energy of the generalized stacking fault (GSF) associated with a rigid shift of one-half of the crystal along some direction in the slip plane. The role of the GSF was introduced by Vitek [29] as an important characteristic for understanding dislocation structure and mobility.

2.1 Cleavage and slip energy barriers for B2 NiAl and FeAl (FLAPW study).

In our first efforts to enhance our understanding of aluminide intermetallics, we investigated the Griffith energies and the unstable stacking fault energies for FeAl and NiAl using the highly precise full potential linearized augmented plane wave (FLAPW) method. Large multilayer relaxation is obtained through atomic force and total energy calculations. The unstable stacking fault energies for $\langle 100 \rangle$ and $\langle 110 \rangle$ slips in NiAl(001) are 1.3 J/m² and 2.2 J/m², respectively. They are much smaller than the tensile cleavage energy, 5.4 J/m², and indicate that the major deformation mode in stoichiometric NiAl is $\langle 100 \rangle$ slip, a result which agrees with experiment. For FeAl(001), the unstable stacking fault energies are much higher and are equally anisotropic (2.4 J/m² and 3.9 J/m² for $\langle 100 \rangle$ and $\langle 110 \rangle$ slips, respectively). We found that $p - d$ hybridization plays an important role at E_F for NiAl but not for FeAl, which may contribute to these different mechanical properties.

2.2 Planar shear and cleavage decohesion processes in NiAl and FeAl (FLMTO study).

An essential feature of the GSF is that as a planar fault, it is not as complicated an object for modeling as is a dislocation, and so it is quite possible to perform accurate ab-initio band-structure calculations of its energetics. On the other hand, what may make it useful is that knowledge of the GSF energetics allows one to analyze the structure of a dislocation core in the scope of the Peierls-Nabarro (PN) model [30, 31] with general restoring force. Thus, the PN model may be considered as a bridge that brings together information offered by ab-initio band structure methods and the problem of dislocation core structure.

We performed for NiAl and FeAl ordered alloys all-electron ab-initio local density calculations of the γ -surface sections and corresponding characteristics of the shear and cleavage decohesion processes. We found that the cleavage energies (G_c) determined with the FLMT0 method are in a good agreement with earlier FLAPW results by Fu and Yoo [33]. The results of our calculations of cleavage characteristics show that both in NiAl and FeAl the habit crack plane is $\{110\}$ which agrees with experimental observations for NiAl. It was shown for a $\text{Fe}_{60}\text{Al}_{40}$ alloy that the $\{100\}$ cleavage plane is preferable [34]. Possible reasons for such a contradiction were discussed by Yoo and Fu [35] and related to a mutual orientation of crack and operative slip planes. The calculated ratio $\mu b/\gamma$ is fairly large (greater than 10), which according to the simple Rice-Thompson criterion indicates a tendency to brittle propagation of the crack in both materials (cf. Sec. IIIA). The same conclusion was also drawn (cf. Sec. IIIB) on the basis of an analysis of the theoretical shear strength, σ_{sh} , and unstable stacking fault, γ_{us} , data. Thus, first-principles calculations show that the mechanism of the intrinsic brittleness both for NiAl and FeAl is likely to be related with a cleavage type of crack propagation. This is consistent with recent experimental studies of the fracture in these intermetallics at room temperature [34, 36]. However, to understand the physical mechanisms driving the difference in tensile ductility of those two alloys one has to address questions not only about crack propagation but also about crack nucleation processes which depends on many factors and first of all on the mobility of dislocations.

Based on ab-initio calculations, the structure of the dislocation cores were determined using solutions of the PN model for a general restoring force. We found that: (i) the core of a $\langle 100 \rangle$ dislocation is compact, in agreement with HRTEM measurement by Mills and Miracle [37]; and (ii) a $\langle 111 \rangle$ dislocation is split into two superpartial $a/2 \langle 111 \rangle$ dislocations. The distance of the splitting in NiAl is about the width of the dislocations, but is much larger in FeAl. Estimates of the Peierls stress in terms of this approach allowed us to reproduce correctly the relation between slip systems ($\langle 100 \rangle \{100\}$ in NiAl and $\langle 111 \rangle \{110\}$ in FeAl). Our calculations and analysis show, in agreement with the original work of Rachinger and Cottrell [38], that the main factor making unlikely the appearance of $\langle 111 \rangle \{110\}$ slip in NiAl is the high APB energy in this alloy, although the shape of the γ -surface also contributes considerably to the structure of the dislocation core. In accordance with our results, compared with NiAl relatively low Peierls stress in FeAl and correspondingly higher mobility of dislocations is likely to be the main intrinsic factor why FeAl shows better tensile ductility than NiAl [34].

3 Ab-initio generalized stacking-fault energetics and properties of dislocations: 1D and 2D PN model analysis with generalized restoring force law

3.1 Dislocation structure and mobility in B2 FeAl and NiAl: 1D PN model analysis with ab-initio GSF energetics.

Despite rather intensive experimental studies, the mechanism of the ductile/brittle properties of B2 intermetallic materials is still far from being well understood and remains a challenge to theoretical explanation. The poor ductility of FeAl is caused mainly by environmental factors (hydrogen-induced embrittlement) [39] in contrast to NiAl which is considered to be intrinsically brittle [40]. However, a recent experiment [36] illustrated that it is possible to achieve high (25%) tensile elongation for high purity monocrystalline NiAl. These experimental facts demonstrate that the nature of the brittleness in this type of material is still not completely understood. In addition it is now well established that these two B2 alloys demonstrate different primary deformation modes ($\langle 100 \rangle \{100\}$ in NiAl and $\langle 111 \rangle \{110\}$ in FeAl [40]). For better understandings of the fundamental factors driving fracture and deformation behaviour of these materials, for the first time for NiAl and FeAl ordered alloys we performed ab-initio calculations of the γ -surface sections and corresponding characteristics of the shear and cleavage decohesion processes. On the basis of these ab-initio calculations, structure of dislocation core were determined using solution of the 1D PN model for general restoring force. The 1D PN model equations were solved in a wide class of analytic function that allowed also to derive expression for Peierls stress in convenient form. structure and Estimates of the Peierls stresses in terms of this approach allowed us to reproduce correctly relation between slip systems ($\langle 100 \rangle (100)$ in NiAl and $\langle 111 \rangle (110)$ in FeAl). Our calculations and analysis show that main factor making unlikely the appearance of $\langle 111 \rangle (110)$ slip in NiAl is the high APB energy in this alloy, although the shape of the γ -surface also considerably contributes to the structure of dislocations core. Our results show that first-principles total energy calculations of γ -surface and shear characteristic in combination with PN model analysis provides reasonable basis for theoretical study of the dislocation structure and operative slip modes for B2 NiAl and FeAl intermetallic compounds.

3.2 Ordinary dislocation properties in TiAl vs. CuAu: Peierls-Nabarro model with two component displacement fields and generalized restoring force law.

The intermetallic alloy γ -TiAl has a number of unique properties which remain at elevated temperatures, including high strength to density ratio, low creep rate and high oxidation resistance. However, full scale applications of this material are limited by low plasticity. In this respect, it is important to stress several experimental facts : (i) a so called temperature anomaly of the yield stress, $\sigma_y(T)$, is detected for monocrystalline TiAl for different crystal orientations in the 600-700° C temperature range [41, 42, 43] and (ii) the plasticity of TiAl is very low (less than 1%) in the wide temperature range up to peak temperature (T_p) and the dependence is sharply increased for $T \geq T_p$. Both of these phenomena are related to the low mobility of dislocations which becomes even lower in the above mentioned temperature anomaly range [44]. Thus, TiAl is essentially different from ordered B2 NiAl and FeAl alloys which have no temperature anomaly and whose deformation behaviour is most probably limited by the presence of light impurities (O,H,C) [40, 39].

It is an intriguing fact that the anomalous $\sigma_y(T)$ dependence is observed for all orientations of the single crystal, including the case when ordinary dislocations determine deformation behaviour. Since the conventional mechanism of dislocation locking (for a review see [45]) is not applicable for ordinary dislocations, the deep and anisotropic Peierls relief (DAPR) hypothesis was formulated to resolve this contradictory situation. This idea was also supported by results of ab-initio charge density calculations which show highly anisotropic covalent character of the chemical bonding in TiAl [46]. The electron microscopy data on the TiAl dislocations structure at different temperatures are also in favor of such a point of view, since sessile single dislocations are observed in the temperature range 200-600 C [47, 44, 43]. However, the nature of the ordinary dislocation low mobility is still unclear.

Thus, a detailed study of the dislocation structure and mobility is essential for a fundamental understanding of the TiAl anomalous mechanical properties. In particular, the problem of the ordinary dislocation in TiAl is especially interesting as a unique example of low dislocation mobility (M) in fcc alloys. As is well-known, high Peierls stress is not typical for the ordinary dislocations in metals and alloys with fcc structure is very small ($\sigma_P/\mu \sim 10^{-4}$). It is important not only to describe the low mobility of a single dislocation but also to explain this feature on the microscopic level in order to provide a theoretical basis for the possible design of new materials with similar structure. It is thus an essential requirement for the theory to address these questions with an accurate description of the covalent character of the chemical bonding in the most accurate way and on this basis to characterize dislocation properties.

Several calculations of the electronic structure and chemical bonding parameters were performed for ordered TiAl [48, 49, 50] and confirmed its strongly covalent character. However, these calculations did not permit an answer to the question whether the DAPR hypothesis is valid or not, since one has to not only characterize chemical bonding but also to establish a relation with dislocation properties. Recently, atomistic simulations with several embedded atom model (EAM) potentials were performed to investigate the structure and mobility of the single dislocation in TiAl [51]. Since the above mentioned directional covalent character of the chemical bonding is missing in the EAM potential, there is a strong motivation for alternative theoretical studies using first-principles methods.

The complexity of the dislocations problem and covalent chemical bonding effects EAM atomistic theoretical approach, namely, Peierls-Nabarro (PN) dislocation model. We thus used a unified scheme (see Sec.1.2.1) for analyzing the dislocation structure and mobility based on solution of the 2D PN model with a two component displacement field and a restoring force law determined from first-principles calculations of the generalized stacking faults (GSF) energetics (ie. the so-called γ -surface). This approach allows first-principles parameterization (γ -surface energetics) which permits the description of covalent directional character of the chemical bonding in an accurate fashion. This theoretical scheme offers the way to characterize dislocation properties qualitatively on the basis of highly accurate first-principles calculations. The approach was applied to investigate the case of realistic, complex situations of dissociated dislocations in γ -TiAl and CuAu. The results of the 2D PN analysis with γ -surfaces, calculated with the FLMTO method using six layer supercells and homogeneous periodic boundary conditions [52, 53] without relaxation for a unit dislocation structure in $L1_0$ TiAl and CuAu show that a unit dislocation in TiAl is compact - in contrast with CuAu [23]. The unit dislocation structure predicted here for TiAl (compact core) is consistent with available experimental data [54] and atomistic simulation results [51] (for an embedded atom potential that gives a value of the CSF energy that is similar to our ab-initio calculations) but our analysis is performed within a highly tractable scheme which allows one to relate qualitative differences in dislocation properties to the ab-initio γ -surface geometry.

We emphasize here the importance of such characteristics that are naturally revealed in our 2D PN model analysis as a "dissociation path" (see Sec.1.2.2) for the understanding of the fracture behaviour within Rice-Thomson (R-T) criteria. As is well-known in the scope of the (R-T) criteria, crack propagation is described by the competition of the crack opening (characterized by the surface energy γ_s) and dislocation emission (characterized by the unstable stacking fault energy γ_{us}) processes. An analysis of this competing process arrives at the criterion of brittle crack propagation, $\gamma_s/\gamma_{us} > 2.9$ [25, 26], which despite its simplicity captures the general tendencies in materials fracture behaviour [26]. Dislocation emission from the crack tip within the R-T criteria is characterized by the energy barrier, γ_{us} . This energy barrier is

usually estimated assuming a straight line "dissociation" path . As we demonstrated above, the actual "dissociation" path may deviate significantly from an assumed straight line. In cases of spread dislocations (CuAu), corresponding changes in γ_{us} estimates are likely to be small but may be quite significant in cases of compact dislocation cores (TiAl). In fact, if features of the actual "dissociation" path are taken into account to determine γ_{us} for TiAl, the R-T criterion ($\gamma_s/\gamma_{us} = 1.7$) predicts brittle crack propagation - opposite to the result which one obtains assuming a straight "dissociation" path ($\gamma_s/\gamma_{us} = 4.5$).

4 Real-space tight-binding-linear-muffin-tin orbital method investigation of point and extended defects in inter-metallics.

4.1 Preferable site energies of impurities in NiAl.

The site preference energy for a number of 3d additions to NiAl has been studied using the real space TB-LMTO-REC method described above. We developed a version of this technique which allows one to calculate the energy of an impurity embedded in an ideal crystal. Results of calculated site preference energies are compared with results of LMTO energy band calculations in Fig. 1. As can be seen, the newly developed method describes the energetics of ternary additions in good agreement with the traditional band structure LMTO-ASA method. The significance of these results is that, in contrast with LMTO-ASA, the real space TB-LMTO-REC method allows one to perform calculations for very low concentrations of additions, and, as described below, can be used to calculate the electronic structure of dislocations and other extended defects . [Preferable site energy in NiAl as calculated by LMTO-ASA method with 16 atom supercell (fill), by TB-LMTO-ASA with supercell (filled) and by TB-LMTO-ASA with single impurity embedded in ideal crystal]

4.2 First-principles calculation of the electronic structure of dislocations: screw and edge dislocations in NiAl.

Electron-dislocation interactions in metallic systems have attracted considerable attention due to a number of experimental results: First, there are those that show a dependence of the electrical resistivity and other kinetic properties on plastic deformations [55, 56, 57]. The correlation between electronic states of impurities and solid-solution hardening observed in

metals and especially in intermetallics [58] may also be treated as an indication of the existence of peculiar states on dislocations which affect dislocation-impurity interactions.

Despite these scientifically and technologically important results, the microscopic mechanisms of electron-dislocation interactions have not been understood for metallic systems. In contrast with semiconductors, the role of "broken" bonds and the deformation potential of a dislocation is not clear in the case of metals.

We recently performed electronic structure calculations of the edge $\langle 100 \rangle$ $\{010\}$ dislocation in NiAl using the real-space tight-binding linear-muffin-tin-orbital recursion (TB-LMTO-REC) method with a self-consistent treatment of the electron density redistribution effects in the dislocation core. We demonstrate that: (i) quasi-localized states may exist as a result of specific lattice distortions in the dislocation core with a type of "broken" bonds; (ii) the electronic structure changes appreciably in the process of dislocation motion; (iii) van-Hove singularities present in the ideal crystal may be shifted to the Fermi level as result of the dipolar character of the deformations in the dislocation core.

5 First-principles calculations of the size misfit parameters for various impurities in NiAl.

First-principles LMTO calculations have been performed to study the electronic structure of NiAl and FeAl doped by Ti, V, Cr, Mn, Fe, Co, Y, La and Zr additions in both sublattices. The preferable sites for ternary additions were found and the sensitivity of preferable site energies from the crystal relaxation effect was investigated. The peculiarities of chemical bonding for both undoped and with some ternary additions in NiAl and FeAl alloys were analyzed using the LMTO-Green function method.

Among the problems actively studied in the B2 intermetallics NiAl and FeAl, the role of impurity dopants on the mechanical behavior of these compounds is of growing interest. Since their mechanical properties depend crucially on microalloying additions, this provides an important tool for controllable alloy design [59]. Particularly important are the attempts to improve creep resistance [60, 61], solid solution hardening (SSH) [60] and the room temperature ductility [62, 63] of NiAl and FeAl.

The mechanism of the ternary addition effects on the mechanical properties of intermetallics is rather complicated and includes the variation of phase equilibrium, vacancy concentration, solubility of interstitial impurities, appearance of anti-site defects, solid solution hardening and others [60]. First of all, however, an alloying atom alters locally the electronic structure and bonding characteristics (bonding directionality, covalency and metalicity of bonds, charge

transfer) which can change the fracture behavior and the ordering type. Especially interesting is the so-called "extra" solid solution hardening phenomenon [59] found in NiAl and Ni₃Al. impurity

The knowledge of preferred sites is very important for understanding differences in the ductility of ternary alloys and for the determination of the degree of solid solution strengthening. Knowledge of the structural relaxation opens a way to estimate a real value of the size misfit parameters while their experimental determination is difficult in the alloys considered [60].

In this work, we determined the electronic structure of NiAl and FeAl doped in both sublattices by the most promising and most frequently investigated additions such as transition (Ti, Cr, V, Mn, Co), refractory (Mo, Zr) and rare-earth (Y, La) metals. We also studied the effect of Fe additions in NiAl and Ni additions in FeAl. Since the experimental and theoretical information about lattice relaxation due to the ternary additions in intermetallics is very limited, we determined the relaxation effects in NiAl. We calculated the site preference energies and then verified the sensitivity of the preference sites to the relaxation. A comparative analysis of chemical bonding was performed for NiAl and FeAl (both undoped and with some additions) using the Green-function LMTO method.

The relaxation effect due to the additives is large for Y, La and Zr, and leads to a decrease of the preferred site energies for these additions. However, it doesn't change the sequence of additives in Table I calculated in the frozen lattice and of course the preferable sublattice. Thus, the preferred sites for the ternary additions is determined mainly by the electronic structure.

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6 References

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Part III

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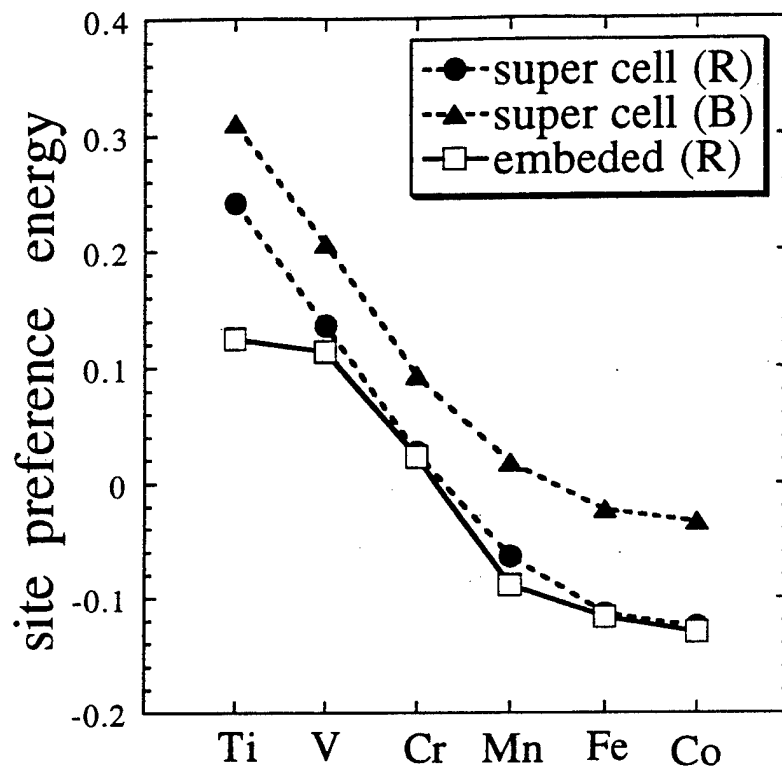


Figure 1: Preferred site energies of the substitutional impurities (Ti,V, Cr, Mn, Fe, Co) in NiAl as calculated by the LMTO-ASA method with 16 atoms in a super cell (super cell (B), filled triangles), by the real space TB-LMTO-REC with the same supercell (super cell (R), filled circles) and by the real space TB-LMTO-REC method with an embedded impurity model (embedded (R), open squares)

TABLE I. The preferable site energies for impurities in NiAl and FeAl

	NiAl	Y	Zr	La	Ti	Mo	V	Cr	Mn	Fe	Co
site	Al	Al	Al	Al	Al	Al	Al	Al	Al	Ni	Ni
$E_{pref}(\text{Ry})$	0.063	0.059	0.047	0.039	0.033	0.026	0.012	0.002	0.002	-0.002	-0.008
	FeAl	Zr	La	Mo	Ti	V	Cr	Mn	Ni	Co	
site	Al	Al	Al	Al	Al	Al	Al	Al	Fe	Fe	
$E_{pref}(\text{Ry})$	0.042	0.038	0.034	0.028	0.025	0.017	0.004	-0.017	-0.017	-0.015	